Testing the Predictive Power of Nuclear-Structure Models Against New Experimental Data

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The mass of a nucleus is one of its most primary properties. Nuclear masses are tabulated in many databases, for example ENDF. In nuclear reaction-rate calculations the Q-value of the reaction is obtained from the nuclear masses of the reaction participants.

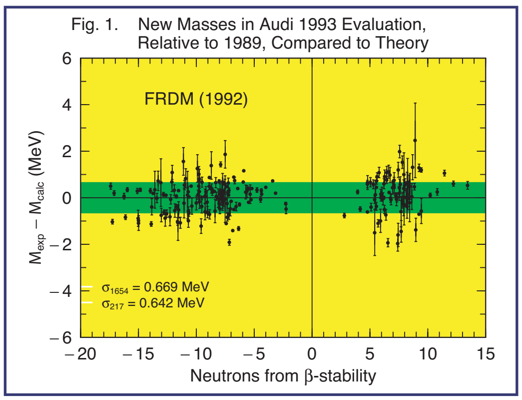

***Figure 1—* Reliability of the FRDM (1992) in new regions of nuclei. The FRDM (1992) was adjusted to 1654 masses known in 1989. The figure shows the deviations between experimental and calculated masses for 217 new nuclei whose masses were measured between 1989 and 1993. The error is 4% smaller in the new region compared with that in the region where the model constants were adjusted. There are no systematic effects visible in the figure.**

In α-decay the half-life of the decay may in many cases be determined to within a factor of 2 or 3 from the decay Q-value alone. At Los Alamos National Laboratory (LANL), nuclear mass models have been developed and refined over a period of about 30 years, starting in the early 1970s. In these models the energy as a function of nuclear shape is calculated as a sum of a macroscopic liquid-drop model energy plus microscopic effects obtained from a deformed single-particle model. Reliable mass models are of paramount importance to provide masses to nuclear databases for nuclei for which no experimental masses are available. A key question is: Are the masses calculated for nuclei where no measurements are available reliable? Or, do the models diverge, as is often assumed, outside the data set to which the model parameters were adjusted? To address this question it is customary to compare published masses obtained from the models of interest to masses that are measured after the publication of the calculations. We argue that in addition one needs to address (1) if the basis of the model is sound, (2) if it is general enough to provide additional nuclear structure quantities, not just nuclear masses, and (3) if the model is global so that it is possible to calculate these properties for any or almost any nucleus with proton number Z and neutron number N. The LANL mass model fulfills these three conditions. The latest version, designated FRDM (1992), was finalized and provided to a limited community in September 1992, submitted for publication in 1993, and published in 1995 [1].

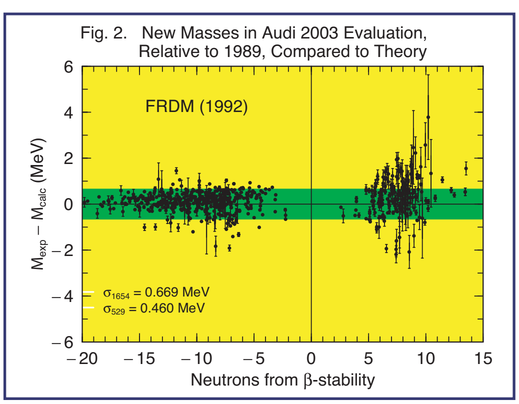

***Figure 2—* Reliability of the FRDM (1992) in new regions of nuclei. The figure shows the deviations between experimental and calculated masses for 529 new nuclei whose masses were measured between 1989 and 2003. The error is 30% smaller in the new region compared with that in the region where the model constants were adjusted. There are no systematic effects visible in the figure.**

The FRDM (1992) model parameters were adjusted to a 1989 interim evaluation of experimental masses by Audi et al. In 1997 we compared the FRDM (1992) masses to 217 masses in a 1993 mass evaluation by Audi et al. that were not present in the 1989 set to which the model was adjusted. Figure 1 shows this comparison; specifically the model error remains constant in this region of new masses. Very recently a new experimental mass evaluation, the Audi 2003 evaluation, became available. This evaluation contains 529 new masses relative to the 1989 evaluation. We show in Fig. 2 the difference between these experimental masses and the corresponding calculated masses. The FRDM (1992) model error in this region of new masses is significantly lower than in the region where the model parameters were determined. Also there is no evidence of any systematic increase in model error with distance from stability. Furthermore we noticed that on the proton-rich side of β stability (negative values of "neutrons from stability") many of the points with the largest deviations in Fig. 1 are not present in Fig. 2! This means that on further evaluation these experimental data points were found incorrect and excluded from the 2003 evaluation!

It has been assumed by some that models that go beyond the single-particle model of the LANL mass model, for example self-consistent Hartree-Fock models based on two-body (Skyrme) interactions, would by nature of their added complexity lead to much better mass models. However, this expectation has so far not been fulfilled. The largest effort in this area is the work by the Brussels group. We compare in Fig. 3 their latest published calculated masses from 2001 (the HFB2 model [2]) to the same set of experimental masses as considered in Fig. 2. The HFB2 model discrepancy with data is much larger than the FRDM (1992) model, *despite* that this 2001 model was *adjusted* to more than 90% of the nuclei in this data set!

The Duflo-Zuker mass model of 1995 [3] is considered by some to show considerable promise. The reason is that the deviation between calculated masses and the 286 new masses measured since the model was presented is only 0.364 MeV, considerably smaller than the FRDM (1992) model error. Also, in their presentation the authors claim it is a "shell model." However, in the end what they do is to fit the parameters of a simple function to data. Consequently one needs to be cautious about its reliability. Moreover it does not fulfill conditions 1 and 2 above.

It is instructive to compare the FRDM (1992), the HFB2, and the Duflo-Zuker mass models to additional experimental quantities. For lack of space we limit our additional comparisons here to the α-decay chain of the new element $^{278}_{113}X$ which was recently observed at RIKEN [4]. It is clear that only the FRDM model shows the characteristic change in slope around $Z = 107–109$, an indication of a deformed stabilizing shell gap

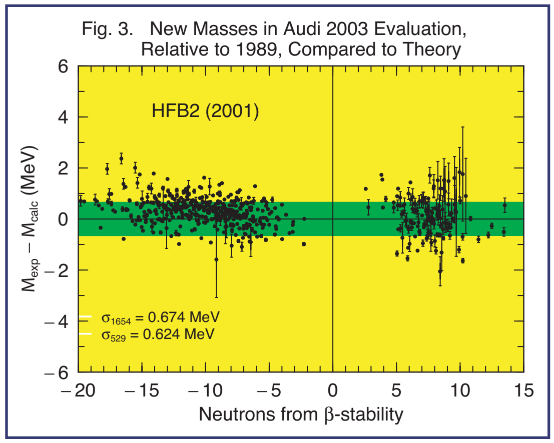

Figure 3—
Comparison of the HFB2 model calculated masses to the same experimental data set considered in Figs. 1–2. Although the HFB2 model was adjusted to more than 90% of the data in this figure [and just as the FRDM (1992) to more than 1600 additional masses known previously] the HFB2 model error is 35% larger than the FRDM (1992) model error in this region.

here. The deviations between data and the Duflo-Zuker model are all of the same sign. This means that the error of this mass model for element $Z = 113$ has grown to 5 MeV.

In summary we have tested the FRDM (1992) mass model and other models against a recently substantially expanded experimental database. In contrast to other models, the FRDM (1992) exhibits extraordinary reliability in the regions of new data. We therefore feel that with considerable confidence we can use this model in LANL databases to provide masses where experimental data are currently unavailable.

[1] P. Möller, et al., *Atomic Data Nucl. Data Tables* **59**, 185 (1995).
[2] S. Goriely, et al., *Phys. Rev. C* **66**, 024326 (2002).
[3] J. Duflo and A.P. Zuker, *Phys. Rev. C* **52**, R23 (1995).
[4] Kosuke Morita, et al., *J. Phys. Soc. Jpn.*, **73**, 2593 (2004).

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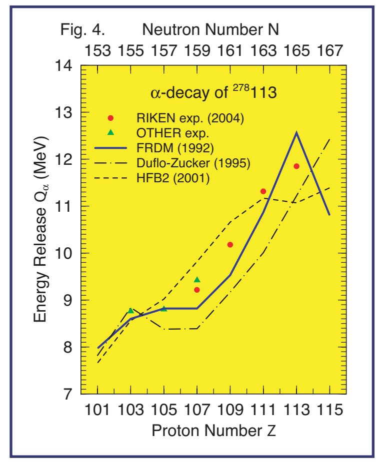

Figure 4—
Observed element $^{278}_{113}X$ α-decay chain compared with three models. The FRDM (1992) best reproduces the characteristic trends in the data that are due to microscopic shell effects.